CC*DNI Engineer: User-centric CyberInfrastructure

Current, Ongoing, and Proposed Projects requiring a CyberInfrastructure Engineer.

Introduction:
Our CyberInfrastructure (CI) Plan emphasizes that UCI is trying to raise both the floor as well as the ceiling in terms of CI. We take our responsibility to the Social Sciences as seriously as to Engineering and are working to encourage all faculty to make use of our aggregate expertise to leverage their research. For example, we are investing time in answering problems in filesharing not only for Terabyte(TB) data sets (via GridFTP and bbcp), but also for small data sets (via OwnCloud).

As described below, we are requesting the CI Engineer (CIE) for a wide variety of tasks, many of which are not generally thought of as being the responsibility of an Engineer. However, the responsibility of an Engineer, is to all of society, not just one segment. This will undoubtedly make finding such a person more difficult, but certainly worth the search. We do not expect to find a single person embodying the expertise required for all these projects, especially since we will be competing against Google, Facebook, EMC, and the like for such talent. However our local support team already has significant expertise in these areas, and we will search for a CIE who has expertise which is compatible and complementary to our own. Each of these projects will be discussed and supported by the Research Computing Support group [1], as well as other local and remote experts in the domain on whom we can call for advice and critique.

Note that we include a number of hyperlinks in this document. These are meant as courtesy references since often the review panel is drawn from groups as heterogeneous as a university faculty and some terms in this document are admittedly obscure. As such, the links are meant only as aids in understanding the flow of the proposal, not as technical references. There are no peer-reviewed citations in this proposal, only documents relating to specific technical aspects.

Following are the projects with which we will task this CIE.

1: Outreach and Consulting with Researchers

There is considerable expertise in our Research Computing Support (RCS) group, which could make a real difference in how researchers deal with data if they realized it was freely available. The CyberInfrastructure Engineer **(**CIE) will endeavor to meet with School and Department heads across campus to alert them to this expertise. If the CIE does not have the expertise to address such problems, she can direct the problems to the rest of the RCS staff which can cooperate to provide answers in the domains of data storage and flow, application-level reconfiguration, algorithms, databases, and even particular applications.

She will also be responsible for writing a monthly newsletter that provides updates CI resources that are available on campus.

Partly in response to the availability and local configurability of the HPC cluster, we have had at least 3 graduate classes being taught with cluster resources, where the students use their own laptops or lab PCs and log into the HPC cluster to run simulations and do symbolic math using the OSS SAGE system. These classes have used all 3 main user interfaces - the web interface, the command line interface, and the X11 graphical interface via the free X11 compression utility x2go (like the VNC or NoMachine clients) We see this as an opportunity to promote cluster computing as a teaching platform as well as a research platform. This may be one of the real advantages of our 10Gbs LightPath network (see below and our CI Plan); to enable the multiple high bandwidth, low-latency connections necessary for fluid GUIs for teaching.
The CIE would also be responsible for reaching out to instructors to make them aware that this extremely cost-effective platform exists and can be integrated into their curriculum.

As well as preaching best practices to researchers at the local institution, the CIE would also have responsibility for outreach to other peer institutions to coordinate conferences (virtual, tele, and actual) to establish relationships, foster information sharing, and even hardware lending to improve overall speed of research. We currently have one XSEDE Campus Champion at UCI, but we would expect her to rise to the point where she would be a natural second one.

While not the primary role of the CIE, she would also engage companies to enable UCI to test or evaluate their technologies to stay ahead of the technology curve. Interacting with such vendors and other researchers about best practices and approaches for data analysis, integrity, tracking, provenance would provide good feedback and 'reality checks' for our own processes.

Implementation

The CIE will attempt to meet with all School and Department Chairs to alert them to the resources on campus, as well as to encourage them to make this known to their faculty. Further, if the Chair allows, we will email his faculty a short note to make them aware of the resources and encourage them to sign up for the monthly update about the resources available. She will create and distribute a monthly email to the faculty list about recent changes in CI and upcoming events that might be of interest.

Milestones

The CIE will contact all Chairs within 1 month of her hire to initiate the process described and will continue to reach out until all School and Department Chairs have been contacted. If they decline to meet, then she will attempt to contact the faculty directly via a single email as above. After that first month, she will send out 1 email per month about CI changes and events. She should also be posting to the relevant listservs: XSEDE, UC-Research-Computing, as well as others that she identifies.

2: LightPath / Science DMZ

UCI was recently awarded a NSF CIE grant to implement a 10Gigabits per second (Gbs) Science DMZ for large data consumers and producers (NSF Proposal # 1341038; DUNS # 046705849).

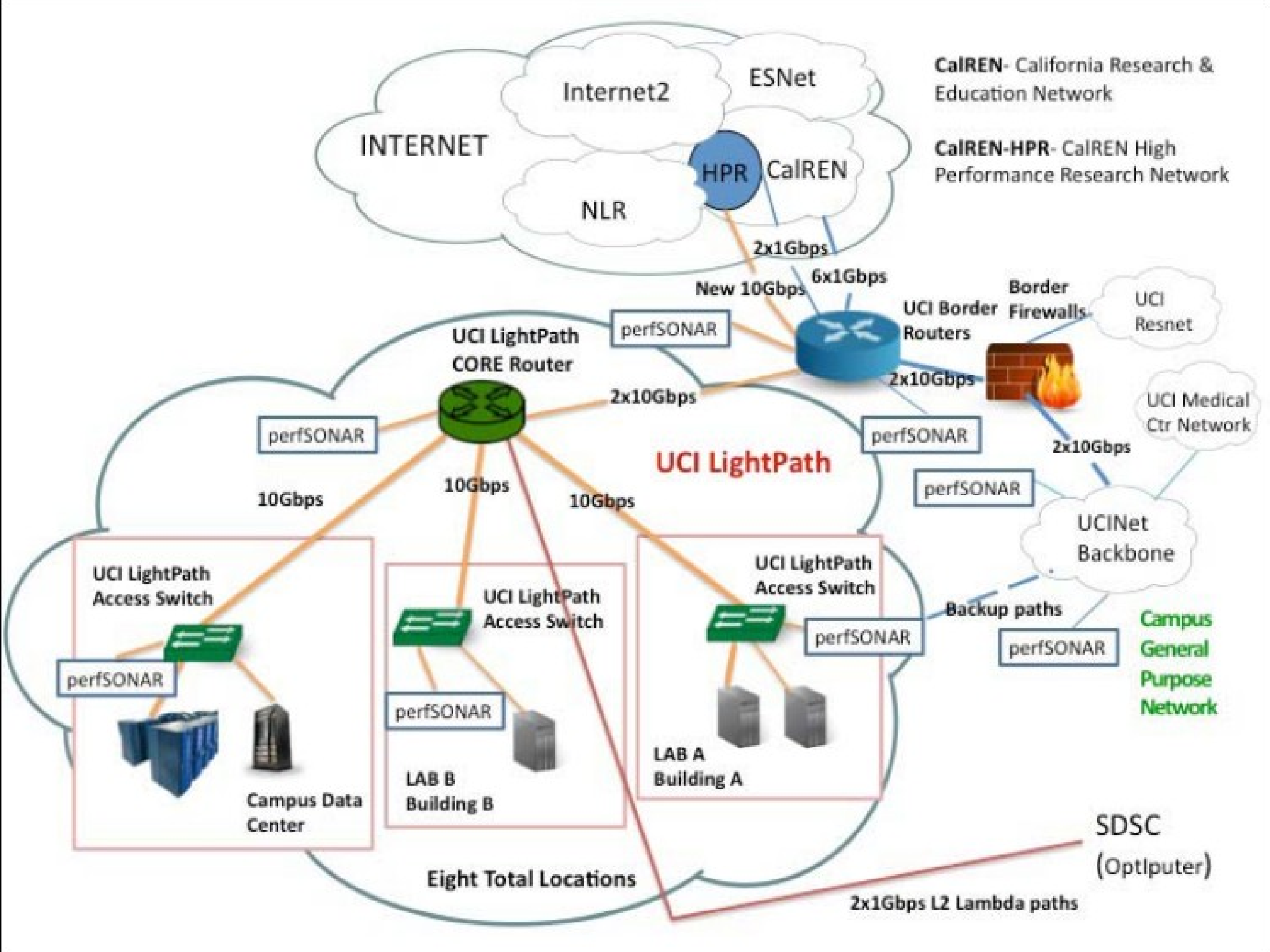
We have purchased, installed, and configured the major equipment, and a few large data sources and sinks have started to use it, but we have yet to get much general uptake due to:

- lack of user education and awareness
- complexity of network configuration
- protocol and port filters block routine tasks (no CIFS/SMB protocols allowed through the firewall preventing 'normal' desktop fileserver access; port blocking on the main firewall masks software licensing requests)
- some user-side security concerns due to concern with lack of a firewall
- few individual systems can supply or digest such very high data rates.
- few compelling interactive applications that require or could exploit such data rates.

UCI's core network is behind a packet-inspecting firewall, unlike the LightPath DMZ (see below)

Figure 1. 10Gbs LightPath Science DMZ relative to UCINet

The diagram below shows how the LightPath DMZ connects to the longhaul internet carriers as well as its relationship to the core UCINet. Note that traffic going to into UCINet must pass a packet-inspecting border firewall, whereas the traffic to LightPath does not; it is protected only by an Access Control List at the Core LightPath Core router (in green in diagram). Diagram courtesy Jessica Yu.



The issues described above are limiting the general uptake of what is a very valuable resource. A CI Engineer would help in both debugging problems and providing documentation on how to do various tasks inside the DMZ.

Examples

- *identifying and configuring a high-bandwidth requiring application that uses a Graphical User Interface, such as VISIT, or one of the 3D image reconstruction applications such as freesurfer.*
- *Connecting, configuring, and teaching how to use a GridFTP client.*
- *Showing users how to use Globus Connect over the LightPath network.*
- *Setting up high-speed Network File System (NFS) mounts to remote sites.*

Implementation

The CIE would assemble and prepare documents describing what our LightPath DMZ is and under what conditions it will be useful to end-users, both using it as part of other resources such as our HPC cluster (which uses it as an high-speed link to external data sources), and as an end-user link if the user has a requirement for high-speed data or low-latency interactions.

If faculty desire further information and/or connection to the LightPath network, she would assist in their determining wiring and hardware requirements and mediating with the Networking group to smooth the process. Once the hardware was in place, and if her documentation was not sufficient to describe how to configure the connection, she would assist in the configuration and modify the documentation to address the problem.

Milestones
The CIE would create an initial document on LightPath within 2 months of hire, and then expand on it in wiki or blog form as more feedback was received or the usage increased, to address each of the points that are mentioned above, with hyperlinks to relevant other institutional documents.

3: Campus Storage Pool

UCI recognizes (and has stated our CI plan) that a key resource for both research faculty and administration is reliable, scalable storage. Previous attempts with such technologies have not been very successful and current commercial products, while viable, tend to be quite expensive when scaling up and like many such products, lead to vendor lock-in and exploitation. There are Open Source, Proprietary, and Hybrid systems available to support this kind of storage pool and this a priority for the CIE. She would to examine and test the options available and provide a written evaluation of such technologies that would be shared with other academic institutions.

We have already dedicated hardware towards this technology evaluation, with a test cluster composed of several older compute and storage nodes with both 1 Gbs Ethernet and Double Data Rate (DDR) Infiniband so as to accurately replicate the working environment, but we lack the time necessary to exploit this resource for extended testing.

We already have some experience with such Distributed File Systems (DFSs) for HPC (Gluster & BeeGFS, and have documented the experience.) and the Campus Storage Pool will have to be some form of DFS. We have to dedicate someone to evaluate a few more before we can responsibly make a decision that will be very long-lived. The DFS that we are now using for our HPC systems (BeeGFS) is quite fast but does not support the kind of failover and reliability that we would need for a storage pool that will be supporting a much wider storage role. The OSS file systems that we would like to test exhaustively are Lustre, DRBD, and possibly Ceph, as well as more testing of these partially (BeeGFS) or completely proprietary (GPFS) filesystems. These testing results will be openly published as we have in the past with our Storage Brick testing and Gluster vs Fraunhofer testing. This is especially important, since there have been very few real-world comparisons of such systems.

Implementation
Once the CIE has been initiated in the dependencies of our existing infrastructure, she will use our existing testbed cluster to test some provisioning technologies and then use the storage servers to test most of the technologies mentioned above, vetting each for various performance metrics (under various loads, with tiny files, streaming, high IOPS, etc), robustness under various failure scenarios, interaction with multiple differing client loads, ease of backups, etc.

Milestones
This is a non-trivial task and one that will probably take at least a year to fulfill with the CIE's other obligations, even with our expertise with clusters and DFSs However, we expect that with assistance, she can run through the provisioning tasks and start producing documents about testing the above filesystems within 3 mo of hire.

4: Hybrid Backup System

Like all institutions, we need robust backup systems to support both our multiple research storage pools and the above-described Campus Storage Pool. 'Single' copies of data are soon 'missing' copies of data. There are certainly commercial systems that can back up storage, but they are all too expensive and lead to exploitive vendor lock-in, as we and others have discovered over the past few years.

We want to design a hybrid tiering backup system that takes advantage of the university's data dynamics to cache recently modified data to a local disk-based system and then forward more stable data to long-term, cheaper storage for archiving. We would like to design the back end for both disk-based and tape-based systems so we can eventually use any pools that are open to us, including Amazon Glacier, UCLA's Cloud Archival Storage Service (CASS), and Univ of Oklahoma's PetaStore. However, the effort to design, code, and implement this system is slower than desired due to lack of human resources.

Implementation
This project is at a very early stage. Besides the use of generic Storage Bricks using ZFS that we would use for the local backup unit, the logic has yet to be written, so the CIE would have fairly wide scope for design choices. Since none of the control logic needs to be especially fast, the logic would probably be an interpreted language like Python or Perl with hooks into bash scripts and the relational database (from the Robinhood Policy Engine that we're already using) for tracking file provenance.
The logic for querying the Robinhood database is fairly easy, and the initial file movement to the local backup unit is trivial, but the logic for the remote transfer may be difficult, especially the business logic, since there are multiple , to connect to a commercial provider
We already have written a parallel rsync application called parsyncfp that can saturate the 10Gbs LightPath network, so pushing the data that fast is not a problem, but deciding which data to push is.
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Milestones
Like the Campus Storage Pool described above, this is a non-trivial task. The CIE will have to come up to speed on a number of CI issues, but since many of them are overlapping (LightPath, the HPC cluster, Distributed File Systems, and the Amazon Elastic Compute Cloud (aka EC2) Application Programming Interface (API), the learning curve should be fairly fast.
We should have a simple proof of concept working within 6 months and a more fully debugged version at the 1 year mark.

5: Dataset Movement, Sync, & Sharing

Data movement is one of the main aggravations in the Big'n'Bigger Data age.   All researchers frequently run into such bottlenecks in moving data to/from endpoints around the world. We have been inspired to write up a fairly well-received document that describes some of the problems and solutions in this domain.

Such bulk data movement is just one of a few related issues. Others are the problem of sharing and syncing data with collaborators and devices. The technology to share a few megabytes back and forth is now hilariously out of date and even Google and DropBox are not reasonable alternatives for multi-TB data sets. We have started to investigate both commercial and OSS solutions as described here.

In order to avoid steep transfer costs charged by commercial services such as Aspera, Signiant, and now even the previously free Globus, research communities have to set up local GridFTP nodes or alternative utilities and educate their users how to use them. This is a non-trivial task, since so many researchers are dependent on Graphical User Interfaces (GUIs) and simple authentication mechanisms, so the idea that you have to use a MyProxy credentialing service is quite foreign, especially via a comand line client.

Implementation
Setting up a solid GridFTP site is non-trivial, and this would be one of the CIE's 1st tasks, since UCI is hosting a 200TB data source for multiple users. She would also be responsible for testing OSS UDP-based file transfer utilities such as tsunami UDP. In any case, UCI must join the ranks of a first class data suppliers as well as

being a first class data consumer.
We are already testing the OSS Owncloud file sharing software to the extent of several TB. For groups of tens of users, it seems to fulfill its promise as a private equivalent to Dropbox but we do not have a good idea of how it scales. The CIE would take responsibility for adding test groups to UCI's local instance and monitoring how well it survives heavy use, software upgrades, and especially the edge cases that academics tend to present.
In addition, she would share authorship of our Data Transfer documents, to be updated as new utilities and protocols are vetted and decided to be useful.

Milestones
While it's non-trivial, it's also well-documented, so setting up a single-host GridFTP site should be completed within 2 months of her hiring. The hardware and networking for a multi-host site is dependent on local funding and other organizations so a full multi-host setup may be delayed for as much as 6 months.
Since there is already a current OwnCloud instance running, there's no setup time for the service, but there will be a short ramp-up while she learns the administration (trivial) and the underlying architecture and performance bottlenecks (non-trivial). She should be fluent in the site administration hours after her first encounter with the interface, but the performance details will certainly not be as simple.

6: Teaching Linux and BigData analytical techniques.

One of the key responsibilities of the CIE will be to accelerate local Linux knowledge and use, especially for large datasets. We have seen some Linux-naive students being asked to analyze TB-sized datasets by similarly naive advisors and they have responded by trying to apply the tools they know - MS Word and Excel, with the expected hilarious/horrendous results. Even those who know their way around Linux are still largely locked in data analysis techniques from a generation ago - the 'grep' and 'cut'-mediated slicing and dicing of columns and rows that were the standard for MB-sized data. Data is now so large that much data is being made available only as compressed binary formats (HDF5, netCDF, XDF, gzipped FASTA, FASTQ) and we need to impress upon researchers in both physical sciences as well as biological ones that this is both a good thing and isn't hard to learn. But without intervention, it's a long, hard path to figuring out how to do this.

In desperation, we have initiated several beginners classes for introducing naive students to Linux and Cluster Computing, bash, Perl, Python, and R programming languages, some popular aspects of Bioinformatics, and BigData. These are not formal computer science classes, but essentially a 'drivers license' for using our compute cluster to protect ourselves against 'drunk data drivers'. These classes are typically one day long, with approximately equal parts lecture and tutorial, the latter done on our HPC cluster.

The CIE would be partly responsible for managing and teaching these classes to the level of her expertise, certainly the 'Introduction to Linux' and the introductory programming classes. She would also be charged with integrating other sources of material into our courses, such as the excellent Software Carpentry series, and the R/BioConductor documentation from Thomas Girke at UC Riverside.

Implementation
Since we already have a basic curriculum, there will be no delay in preparing content, but there will be delay as the CIE is introduced to the class, first as a spectator and then as a co-instructor, and finally as a solo instructor. She will then be expected to expand various aspects of the course in both lecture and tutorial aspects, coordinating with the other classes on R, and BigData.

Milestones
The CIE will attend the first classes given as soon as she is hired, and will be expected to help out as a tutorial assistant at that point. Since the courses are given about every 2 months, she should be ready to co-instruct the class after that and to teach it solo after that. Simultaneously, she should be creating content to address missing topics, such as more advanced (but still quite basic) programming using scripting languages, understanding and

using the SGE scheduler, profiling and debugging code.

7: Cluster Cloudbursting

Cloudbursting is the use of a public cloud service to address overloads in private cloud processing. It is not a novel idea, but marshaling the necessary logic and network channels to support and integrate it into our systems is a non-trivial task. We plan to use it to offload highly compute-bound tasks running on our HPC cluster, if the user is amenable to paying real dollars for the acceleration. In many situations, a group has not spent the ~$10,000 to purchase a large compute node for the cluster, but still needs jobs to run at at accelerated pace. Even though the HPC Cluster scheduler is highly efficient and we use checkpointing and cycle scavenging to provide as much efficiency as possible, it is becoming a victim of its own popularity

Using our cluster scheduler, this would not be possible, but if the PI was willing to set up an Amazon EC2 account, she could bypass the priority settings on our cluster and run much faster on a virtual cluster on Amazon EC2. Our part would be to provide the logic so that this would be transparent to the user.

Using the Distributed Resource Management Application API (DRMAA) for our local cluster resource manager (which is Son of Grid Engine (SGE), an OSS Sun Grid Engine descendant), we expect the CIE to create the programming logic to offload some of our current local compute load to remote resources like Amazon's EC2 for those jobs that are primarily compute-bound. Jobs that are disk-bound would stay local where our DFS is optimized to handle that load, but code for compute-intensive jobs such as complex simulations, iterative sampling, etc could be transferred to a remote system (commercial or academic) for execution and as long as the output was reasonably sized (a key criteria, since many service providers charge considerably for data egress), the output could be transparently and economically returned to our cluster storage. This would require SGE setup and integration with Amazon's EC2 as well as Google's AppEngine. Other people here have very deep experience with SGE so that part of it is mostly covered. Digging through the different APIs and especially figuring out the charging models will be much more complex.

Implementation

Since we use Son of Grid Engine, which has built-in support for the DRMAA, we have to 'spin up' an SGE cluster instance in whatever cloud we want to burst into and enable the appropriate DRMAA channels to accept our request. Like many such technologies, the actual technology isn't the problem so much as the administration surrounding the technology. In this case, getting and setting the billing information for the user, and then making sure all the notifications are made before a simple bash mistake causes thousands of dollars in billing is non-trivial. It may even be non-viable if the downsides and complexity exceed the upsides. Nevertheless, the potential upsides could be quite high, since this would allow significant expansion of our cluster's apparent power with a reduction in Data Center space and energy use.

Milestones

This is a secondary task, so it would probably not be started until 6mo after the hire, until the CIE has learned a significant amount about all the dependent technologies and our implementation of them. Like many such projects, this would require considerable research, prototyping and trial and error to work out how the API calls actually translate to actions. We expect that a proof of concept or a document detailing that is is not worth pursuing is about 1 year away from hire.

8: Sustainability

For Dana/Hemminger to fill out.

9: References

[1] The Research Computing Support group consists of 3.5 FTEs and one exceptional student.

Harry Mangalam, PhD (UCSD), one of the coPIs of this grant, and whose Biosketch is included in the proposal.

Joseph Farran, an experienced systems administrator and programmer whose expertise with cluster computing in all its facets has contributed to making the HPC cluster the largest and fastest growing research compute facility at UCI, and with 900 post-graduate users from all Schools, one of the most widely used research facilities at UCI, period. He single-handedly integrated the Berkeley Lab Checkpoint/Restart checkpointing into our scheduler system and enhanced it with the CPU-scavenging system that allows all users to effectively gain more resources than they paid for.

Tony Soeller, an expert on Geographical Information Systems, whose talents have advanced a number of UCI research programs that depend on geolocation and integration with geographic data sources. He has also been key to fostering interactions with the Faculty Research Computing and Networking Advisory Group mentioned in our CI plan that assures faculty oversight of CI resources.

Garr Updegraff, PhD (UCSD), a ½ time programmer and extraordinary database expert, who wrote much of UCI's Registrar's system and who we are lucky to have on staff due to his interest in research problems and algorithms. He was going to retire until we were able to retain him by offering him this ½ time position which was much more engaging and challenging.

Edward Xia, an undergrad Information & Computer Science student assistant who has such a tireless work ethic and cutting curiosity about all things digital that he is teaching us as much about modern web programming and data techniques as we are teaching him about cluster and high performance computing.